

INVENTOR SEARCH

=> fil casre; d que nos l30

FILE 'CASREACT' ENTERED AT 11:19:12 ON 13 DEC 2007

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FILE CONTENT:1840 - 8 Dec 2007 VOL 147 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 13.8 million reactions
*
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L7          STR
L10         STR
L11         STR
L12         STR
L13         STR
L14         STR
L15         STR
L18         1017 SEA FILE=CASREACT SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR
              L15) NOT L7 ( 7766 REACTIONS)
L19         957 SEA FILE=CASREACT ABB=ON L18/COMPLETE
L21         29 SEA FILE=CASREACT ABB=ON SHCHERBAKOVA I?/AU
L22         0 SEA FILE=CASREACT ABB=ON BALANDRIA M?/AU
L23         101 SEA FILE=CASREACT ABB=ON HUANG G?/AU
L24         5 SEA FILE=CASREACT ABB=ON GEOFFROY O?/AU
L25         116 SEA FILE=CASREACT ABB=ON FOX J?/AU
L26         50 SEA FILE=CASREACT ABB=ON NAIR S?/AU
L29         7 SEA FILE=CASREACT ABB=ON BALANDRIN M?/AU
L30         3 SEA FILE=CASREACT ABB=ON (L21 OR L22 OR L23 OR L24 OR L25 OR
              L26 OR L29) AND L19
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=> d ibib abs fh1t l30 1-3

L30 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:59927 CASREACT Full-text

TITLE: Design, new synthesis, and catalytic activity of substituted 3H-pyrimidin-4-ones

AUTHOR(S): Shcherbakova, Irina; Huang, Guangfei
; Geoffroy, Otto J.; Nair, Satheesh

K.; Swierczek, Krzysztof; Balandrin, Manuel
 F.; Fox, John; Heaton, William L.;
 Conklin, Rebecca L.

CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake
 City, UT, 84108, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),
 15(10), 2537-2540

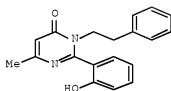
CODEN: BMCLE8; ISSN: 0960-894X

Elsevier B.V.

PUBLISHER: Journal

DOCUMENT TYPE: English

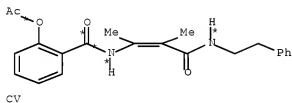
GI



I

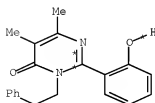
AB Design, synthesis, structure-activity relationship studies and calcium
 receptor antagonist (calcilytic) properties of 3H-pyrimidin-4-ones, e.g., I,
 are described. The pyrimidinones were synthesized by multistep procedures.

RX(80) OF 424 ...CV ==> DH



CV

(80)
 →



DH
 YIELD 70%

RX(80) RCT CV 780771-39-3
 RGT U 1310-58-3 KOH
 PRO DH 780771-35-9
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 12 hours, reflux

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:379934 CASREACT Full-text
 TITLE: Preparation of 2,3,5,6-tetrasubstituted
 3H-pyrimidin-4-ones via cyclization of carboxamides.

INVENTOR(S): Shcherbakova, Irina; Balandrin,
 Manuel; Huang, Guangfei; Geoffroy,
 Otto; Fox, John; Nair, Sathesh
 K.

PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

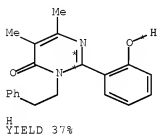
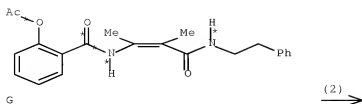
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------|
| WO 2004092121 | A2 | 20041028 | WO 2004-US10639 | 20040407 |
| WO 2004092121 | A3 | 20050414 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| EP 1613606 | A2 | 20060111 | EP 2004-749815 | 20040407 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR | | | |
| JP 2006522160 | T | 20060928 | JP 2006-509759 | 20040407 |
| US 2007161792 | A1 | 20070712 | US 2006-551920 | 20061120 |
| PRIORITY APPLN. INFO.: | | | US 2003-460859P | 20030407 |
| | | | US 2003-479323P | 20030618 |
| | | | WO 2004-US10639 | 20040407 |

OTHER SOURCE(S): MARPAT 141:379934

AB The title process is claimed. Thus, 3-(2-acetoxybenzoylamino)-2-methylbut- 2-enoic acid phenethylamide (preparation given) was refluxed overnight with KOH in EtOH/H₂O to give 37% 2-(2-hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one.

RX(2) OF 57 ...G ==> H



RX(2) RCT G 786771-39-3

STAGE(1)

RGT I 1310-58-3 KOH
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON SUBSTAGE(1) overnight, reflux
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON pH 1

PRO H 786771-35-3

L30 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 141:366249 CASREACT Full-text
 TITLE: Preparation of pyrimidinone compounds as calcilytics
 INVENTOR(S): Shcherbakova, Irina V.; Balandrin,
 Manuel F.; Huang, Guangfai;
 Geoffroy, Otto; Foz, John; Marquis,
 Robert; Yamashita, Dennis Shinji; Luengo, Juan; Wang,
 Wenying
 PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA; Glaxosmithkline
 SOURCE: PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| WO 2004092120 | A2 | 20041028 | WO 2004-US10638 | 20040407 |

WO 2004092120 A3 20050414

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004230903 A1 20041028 AU 2004-230903 20040407

CA 2521129 A1 20041028 CA 2004-2521129 20040407

EP 1615897 A2 20060118 EP 2004-749814 20040407

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

CN 1835928 A 20060920 CN 2004-80009255 20040407

JP 2006522159 T 20060928 JP 2006-509758 20040407

MX 2005PA10683 A 20060801 MX 2005-PA10683 20051004

US 2007197555 A1 20070823 US 2006-552363 20061120

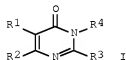
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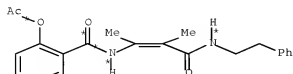
OTHER SOURCE(S): MARPAT 141:366249

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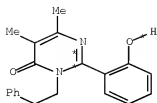
AB Title compds. I [R1-2 = H, halo, CN, CF3, etc.; R3 = aryl; R4 = H, alkyl, etc.] are prepared For instance, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one is prepared from o-hydroxybenzoxonitrile, acetyl chloride and Me acetoacetate. Compds. of the invention have IC50 values < 30 μ M in a calcium receptor inhibition assay. I are useful for the treatment of abnormal bone or mineral homeostasis.

RX(5) OF 72 ...Q ==> P



Q

(5) →



R
YIELD 37%

RX(5) RCT Q 780771-39-3

STAGE(1)

RGT S 1310-58-3 KOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) overnight, reflux
SUBSTAGE(2) cooled

STAGE(2)

RGT K 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

PRO R 780771-35-9

REACTION SEARCH

=> fil casre; d stat que 135; d stat que 140; s 135,140 not 130
 FILE 'CASREACT' ENTERED AT 11:19:46 ON 13 DEC 2007
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FILE CONTENT:1840 - 8 Dec 2007 VOL 147 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 13.8 million reactions   *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L7 STR

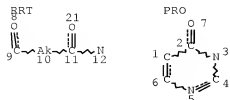


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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
 L10 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

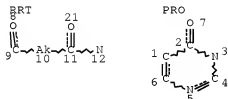
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 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

MAPPINGS

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|-----|-----|-----|-----|-----|-----|
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| 12 | N | RRT | 3 | N | PRO |

L11 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

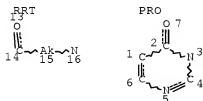
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STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
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| 12 | N | RRT | 5 | N | PRO |

L12 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

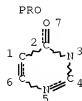
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 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

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|---------|-----|---------|-----|
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| 16 N | RRT | 3 N | PRO |

L13 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

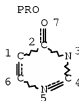
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STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
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| 16 N | RRT | 5 N | PRO |

L14 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

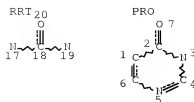
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STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
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L15 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

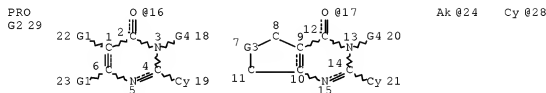
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STEREO ATTRIBUTES: NONE

MAPPINGS

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|---------|-----|---------|-----|
| 5 N | PRO | 19 N | RRT |
| 19 N | RRT | 5 N | PRO |

L18 1017 SEA FILE=CASREACT SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR
 L15) NOT L7 (7766 REACTIONS)
 L31 STR



L35 13 SEA FILE=CASREACT SUB=L18 SSS FUL L31 (67 REACTIONS)
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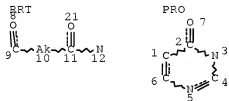
L7 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
 L10 STR



NODE ATTRIBUTES:
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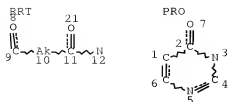
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STEREO ATTRIBUTES: NONE

MAPPINGS

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L11 STR



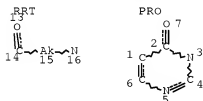
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 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
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| 5 N | PRO | 12 N | RRT |
| 12 N | RRT | 5 N | PRO |
| L12 | STR | | |



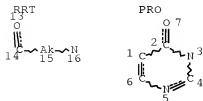
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STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
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| 16 N | RRT | 3 N | PRO |
| L13 | STR | | |



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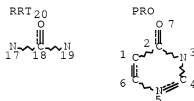
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 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

MAPPINGS

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|-----|-----|-----|-----|-----|-----|
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L14 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

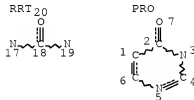
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STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
| 3 | N | PRO | 19 | N | RRT |
| 19 | N | RRT | 3 | N | PRO |

L15 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 11

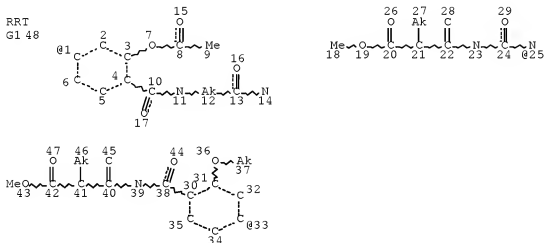
STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 5 N | PRO | 19 N | RRT |
| 19 N | RRT | 5 N | PRO |

L18 1017 SEA FILE=CASREACT SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR L15) NOT L7 (7766 REACTIONS)

L37 STR



VAR G1=1/25/33

NODE ATTRIBUTES:

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 CONNECT IS E1 RC AT 27
 CONNECT IS E1 RC AT 37
 CONNECT IS E1 RC AT 46
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 12
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L40 4 SEA FILE=CASREACT SUB=L18 SSS FUL L37 (13 REACTIONS)

100.0% DONE 87 VERIFIED 13 HIT RXNS 4 DOCS
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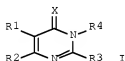
L46 10 (L35 OR L40) NOT L30

=> d ibib abs fh1t l46 1-10; fil hom

L46 ANSWER 1 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 143:477975 CASREACT [Full-text](#)

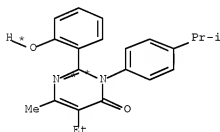
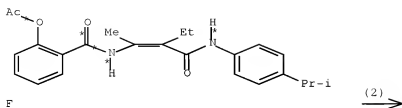
TITLE: Preparation of pyrimidinones and quinazolinones as calcilytic compounds
 INVENTOR(S): Luengo, Juan I.; Marquis, Robert W., Jr.; Xie, Ren; Yamashita, Dennis S.
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-------------------|----------|
| WO 2005108376 | A1 | 20051117 | WO 2005-US15224 | 20050503 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1742924 | A1 | 20070117 | EP 2005-744198 | 20050503 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV | | | | |
| US 2007232628 | A1 | 20071004 | US 2006-568709 | 20061106 |
| PRIORITY APPLN. INFO.: | | | US 2004-568585P | 20040506 |
| | | | WO 2005-US15224 | 20050503 |
| OTHER SOURCE(S): | | | MARPAT 143:477975 | |
| GI | | | | |



AB The title compds. I [R1, R2 = H, halo, CN, etc.; or R1 and R2 may be bonded together to form a carbocyclic, heterocyclic, aryl or heteroaryl ring; R3 = aryl or heteroaryl group which may have 1-5 substituents each selected from H, halo, CN, CF₃, etc.; R4 = aryl which may have 1-3 substituents consisting of H, halo, CN, CF₃, etc.; X = O or S], useful for treating a disease or disorder characterized by an abnormal bone or mineral homeostasis, were prepared E.g., a multi-step synthesis of 2-(2-hydroxyphenyl)-3-(4-isopropylphenyl)-5,6,7,8-tetrahydro-3H-quinazolin-4-one, starting from Et 2-aminocyclohex-1-enecarboxylate and 2-benzoyloxybenzoyl chloride, was given. The methods for treating diseases or disorders such as osteosarcoma, periodontal disease, fracture healing, osteoarthritis, joint replacement, rheumatoid arthritis, Paget's disease, humoral hypercalcemia, malignancy and osteoporosis by administering the compound I alone or in combination with anti-resorptive agents are disclosed.

RX(2) OF 83 ...F ==> G



RX(2) RCT F 920264-52-4

STAGE(1)

RGT H 1310-58-3 KOH

SOL 7732-18-5 Water, 64-17-5 EtOH

CON SUBSTAGE(1) 5 hours, room temperature -> reflux

SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RGT I 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature, pH 1

PRO G 869564-58-9

REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 112:55906 CASREACT [Full-text](#)

TITLE: Process for preparing 4-hydroxypyrimidines as drug and agrochemical intermediates

INVENTOR(S): Ataka, Kikuo; Omori, Kiyoshi

PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 10 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

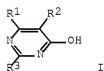
English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|------|----------|-----------------|----------|
| EP 326389 | A2 | 19890802 | EP 1989-300768 | 19890126 |
| EP 326389 | A3 | 19911113 | | |
| EP 326389 | B1 | 19960911 | | |
| R: CH, DE, FR, GB, IT, LI | | | | |
| JP 01279874 | A | 19891110 | JP 1988-323436 | 19881223 |
| JP 06025157 | B | 19940406 | | |
| US 4935516 | A | 19900619 | US 1989-300612 | 19890123 |
| | | | JP 1988-17239 | 19880129 |

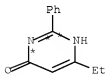
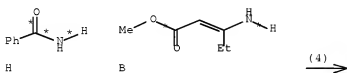
PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 112:55906
GI



AB The title compds. I (R1, R2 = H, C1-10 alkyl, C3-10 cycloalkyl, etc.; R3 = C7-10 alkyl, C3-10 cycloalkyl, etc.), useful as drug and agrochem. intermediates, were prepared by condensation of aminoalkenoates with amides. A mixture of Me 3-amino-2-pentenoate, HCONH2, and MeONa was heated for 3 h at 110° to give 91.9 mol% 6-ethyl-4-hydroxypyrimidine.

RX(4) OF 6 H + B ==> I

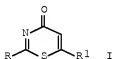


YIELD 81%

RX(4) RCT H 55-21-0, B 124413-61-2
PRO I 82501-10-4

L46 ANSWER 3 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

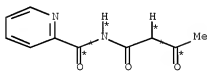
ACCESSION NUMBER: 100:6431 CASREACT Full-text
 TITLE: 1,3-Oxazines and related compounds. VI. Synthesis
 and some reactions of 2,6-disubstituted
 4H-1,3-thiazin-4-ones
 AUTHOR(S): Yamamoto, Yutaka; Ohnishi, Shuhei; Azuma, Yutaka
 CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, 983, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1983), 31(6),
 1929-35
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



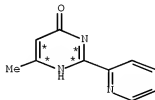
AB 2,6-Disubstituted 4H-1,3-thiazin-4-ones I (R = alkyl, Ph, pyridyl; R1 = alkyl, CH2Ph) were synthesized by successive treatment of RCONHCOCH2COR1 with acid, such as 70% HClO4 or FSO3H and H2S. Ammonolysis of I with NH3-EtOH gave the corresponding pyrimidin-4-ones; hydrolysis of 2-alkyl-1,3-thiazine derivs. yielded RCONHCOCH:CR1SH reduction with NaBH4 or LiAlH4 afforded 3,4-dihydro-2H-1,3-thiazin-4-one derivs.

RX(62) OF 63 COMPOSED OF RX(26), RX(10)

RX(62) BA ==> AE



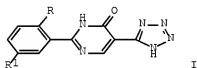
2
STEPS
→



RX(26) RCT BA 82437-55-6
 RGT M 7783-06-4 H2S, H 497-19-8 Na2CO3, N 7789-21-1 HSO3F
 PRO Y 88136-80-5
 CAT 144-55-8 NaHCO3
 RX(10) RCT Y 88136-80-5
 RGT Q 1336-21-6 NH4OH
 PRO AE 55417-80-6

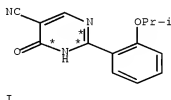
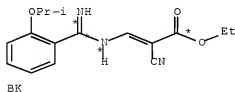
CAT 64-17-5 EtOH

L46 ANSWER 4 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 97:155925 CASREACT Full-text
 TITLE: Antiallergy agents. 2. 2-Phenyl-5-(1H-tetrazol-5-yl)pyrimidin-4(3H)-ones
 AUTHOR(S): Juby, Peter F.; Hudyma, Thomas W.; Brown, Myron; Essery, John M.; Partyka, Richard A.
 CORPORATE SOURCE: Bristol Lab., Div. Bristol-Myers Co., Syracuse, NY, 13201, USA
 SOURCE: Journal of Medicinal Chemistry (1982), 25(10), 1145-50
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB I (R = alkoxy, OCH₂CH₂CH₂, or cyclopropylmethoxy; R₁ = H, OMe, NO₂, NH₂, or NMe₂) were prepared and found to be about 5-10 times more potent than the corresponding pyrimidine-5-carboxylic acids when tested orally against passive cutaneous anaphylaxis in the rat. Structure-activity relations within the two series are similar. I (R = OPr, R₁ = H) [64634-09-9] is in clin. trial for the prophylactic treatment of asthma.

RX(38) OF 80 BK ==> I...



RX(38) RCT BK 64634-07-7
 PRO I 64661-66-1
 SOL 67-68-5 DMSO

L46 ANSWER 5 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 97:55759 CASREACT Full-text
 TITLE: Studies on 1,3-benzoxazines. VII. Formation of diphenylpyrimidines by the reaction of

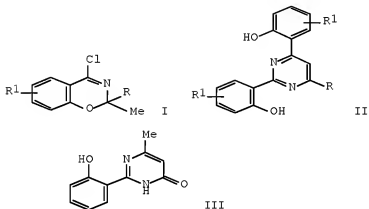
4-chloro-2H-1,3-benzoxazines with ethyl
3-aminobutyrate

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

Tachikawa, Ryuji; Wachi, Kazuyuki; Terada, Atsuke
Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan
Chemical & Pharmaceutical Bulletin (1982), 30(2),
564-8

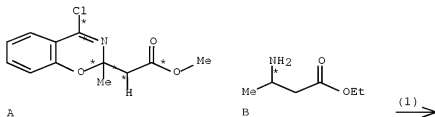
DOCUMENT TYPE:
LANGUAGE:
GI

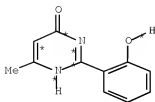
CODEN: CPBTAL; ISSN: 0009-2363
Journal
English



AB Treatment of chlorobenzoxazines I (R = Me, R1 = H, 5-MeO, 4-Cl, 5-Cl; R = Et, R1 = H; R = Ph, R1 = H) with H2NCHMeCH2CO2Et gave pyrimidine derivs. II. When 4-chloro-2-methyl-2-methoxycarbonylmethyl-2H-1,3-benzoxazine was treated with H2NCHMeCH2CO2Et, a pyrimidine derivative III was isolated. A possible mechanism for the formation of these reaction products is discussed.

RX(1) OF 5 ...A + B ==> C





C

RX(1) RCT A 82507-98-0, B 5303-65-1
PRO C 76467-22-6

L46 ANSWER 6 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 95:24980 CASREACT [Full-text](#)

TITLE: Reaction of 3-aminocrotonamide with nitriles

AUTHOR(S): Kato, Tetsuzo; Chiba, Takuo; Sasaki, Makoto

CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan

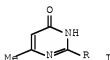
SOURCE: Heterocycles (1981), 16(4), 577-80

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

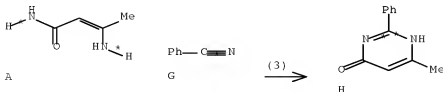
GI



I

AB Reaction of 3-aminocrotonamide with RCN (R = Me, Et, Me₂CH, Ph) in MeOH in the presence of NaOMe gave I (same R) in 18-44% yields. Also, reaction of PhCH₂CN with 3-aminocrotonamide gave 2-benzyl-6-methyl-4(3H)-pyrimidinone and 6-amino-4-methyl-5-methyl-2(1H)-pyridone. Reaction of malononitrile with 3-aminocrotonamide gave 6-amino-5-cyano-4-methyl-2(1H)-pyridone.

RX(3) OF 7 A + G ==> H



RX(3) RCT A 15846-25-0, G 100-47-0
PRO H 13514-79-9

CAT 124-41-4 NaOMe

L46 ANSWER 7 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 91:39426 CASREACT Full-text

TITLE: Synthetic plant growth regulators. The synthesis of C-o-carboxyphenyl derivatives of pyrimidine

AUTHOR(S): Harris, Roger L. N.; Huppertz, John L.; Teitei, Tsutomu

CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, 2601, Australia

SOURCE: Australian Journal of Chemistry (1979), 32(3), 669-79

CODEN: AJCHAS; ISSN: 0004-9425

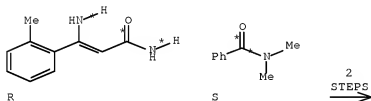
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthetic routes to o-carboxyphenyl derivs. of pyrimidine, required for testing as potential plant growth regulators, are described. 2-(4-Phenylpyrimidin-2-yl)benzoic acid, 2-(2-phenylpyrimidin-4-yl)benzoic acid, and 2-(2-phenylpyrimidin-5-yl)benzoic acid were prepared by utilizing amide-acid chloride intermediates in the generation of the pyrimidine ring in each instance.

RX(34) OF 57 COMPOSED OF RX(10), RX(12)

RX(34) R + S ==> U



U
YIELD 25%

RX(10) RCT R 70484-37-6, S 611-74-5
PRO Q 70484-36-5

RX(12) RCT Q 70484-36-5
RGT K 10588-01-9 Na2Cr2O7
PRO U 343623-34-9

L46 ANSWER 8 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 87:5899 CASREACT Full-text

TITLE: Pyrimidines. LIX. Ring transformations of heterocyclic compounds with nucleophiles. Part XVI. Degenerate ring transformations of 1,3-diethyl-1,4(3,4)-dihydro-4-oxopyrimidinium tetrafluoroborates with ammonia

AUTHOR(S): Oostveen, E. A.; Van der Plas, H. C.

CORPORATE SOURCE: Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, Neth.

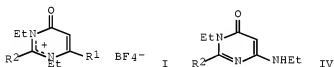
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1977), 96(3), 68-72

CODEN: RTCFA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

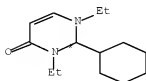
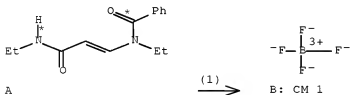
LANGUAGE: English

GI



AB Treatment of the pyrimidinium tetrafluoroborates I ($R_1 = H, Me, Ph, OEt$; $R_2 = H, Ph, Me$) with aqueous NH_3 or $NH_3(l)$ gave $R_2CONEtCOCH:CR_1NH-Et$ (II) and $EtNHCOCH:CR_1NEtCOR_2$ (III) via cleavage of the $N(1)-C(2)$ or $N(3)-C(2)$ bond, resp. However, in the case of I ($R_1 = OEt$), II or III recycled with $NH_3(l)$ with elimination of $EtOH$ to give the ethylaminopyrimidinones IV.

RX(1) OF 17 ...A ==> B



B: CM 2

RX(1) RCT A 343879-52-7
 PRO B 62880-85-1
 CAT 16872-11-0 HBF4

L46 ANSWER 9 OF 10 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 66:55438 CASREACT Full-text

TITLE: Reactions with trifluorochloroethylene. II. Addition of trifluorochloroethylene to imidazole, benzimidazole, and naphthimidazole--a new cleavage of the imidazole ring

AUTHOR(S): Ried, Walter; Lohwasser, Hermann

CORPORATE SOURCE: Univ. Frankfurt, Frankfurt, Germany

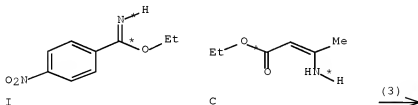
SOURCE: Justus Liebigs Annalen der Chemie (1966), 699, 88-97
 CODEN: JLACBF; ISSN: 0075-4617

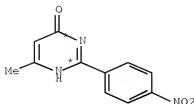
DOCUMENT TYPE: Journal

LANGUAGE: German

AB cf. CA 66, 28568c. The title compds. were alkylated on the N atom by CF₂:CClF (I) under pressure at elevated temps. without a catalyst. The trifluorochloroethyl group makes the imidazole ring of the 1:1 adducts accessible to nucleophilic attack, which leads to a ring cleavage. A novel aldehyde synthesis and a triazole synthesis are described. The alkylations with I without catalyst proceeded in a few hrs. at temps. over 100° under the vapor pressure of the solution in absolute tetrahydrofuran (THF). Expts. with 10-80 g. compound were carried out in a 0.5-l steel autoclave. Into the reaction chamber precooled with dry ice were introduced the intensely cooled solvent, the reacting compound with some hydroquinone, and the weighed liquefied I together with the cooling trap used for the condensation, in to bind the liberated HF from side reactions. On heating the autoclave, the pressure did not rise above 30 kg./cm.² Benzimidazole (35 g.), 200 cc. THF, and 53 g. I heated 5 hrs. at 130-40° gave 61 g. N-(1,1,2-trifluoro-2-chloroethyl)benzimidazole.

RX(3) OF 3 I + C ==> J





J
YIELD 69%

RX(3) RCT I 831-68-5, C 626-34-6
PRO J 13514-80-2
SOL 7732-18-5 Water
NTE Classification: Heterocycle formation; Condensation;
Isomerisation; C-Amination; # Conditions: H2O 50-60 deg 2 days

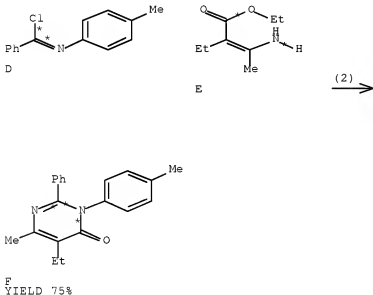
L46 ANSWER 10 OF 10 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 51:39274 CASREACT Full-text
TITLE: Synthesis of 2,3,5,6-substituted 4-pyrimidones
AUTHOR(S): Staskun, Benjamin; Stephen, Henry
CORPORATE SOURCE: Univ. Witwatersrand Johannesburg, S. Afr.
SOURCE: Journal of the Chemical Society (1956) 4/08-10
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 2,3,5,6-Substituted 4-pyrimidones (I) were readily synthesized by condensation of imidoyl chlorides (II) with Me or Et α -alkyl- β -aminocrotonates (III). The following general procedure was used: II (0.01 mole) and III (0.005, 0.01, or 0.02 mole) were refluxed 3-4 hrs. in 40 cc. dry CHCl₃ (method A) or allowed to remain at room temperature 2-3 days (method B). In some cases II and III were heated in the absence of a solvent (method C), HCl and alc. being evolved. The products were acidified with dilute HCl and steam distilled; this hydrolyzed any unchanged ester to steam volatile or H₂O soluble products, and converted unchanged II to the amide. After cooling, the latter was removed, and the filtrate treated with C and NH₃ deposited crude I which crystallized from dilute MeOH or alc. in colorless needles. The following I were prepared by the above methods (R and R' substituents in II (RCCL:NR'), R' and X in III (MeC(NH₂):CR''CO₂X), molar ratio II:III, method, reaction temperature, reaction time in hrs., % yield, and m.p. given): Ph, Ph, Me, Me, 1:1, C, 140°, 0.5, -, -, Ph, Ph, Me, Et, 1:1, C, 140°, 0.5, 45, 157°; Ph, Ph, Et, Et, 1:2, A, -, 4, 79, 159°; Ph, o-C₆H₄Me, Me, Me, 1:1, A, -, 3, 53, 114°; Ph, o-C₆H₄Me, Et, Et, 1:2, A, -, 4, 80, 152°; Ph, m-C₆H₄Me, Me, Me, 1:1, C, 100°, 0.5, 31, 129°; Ph, m-C₆H₄Me, Me, Et, 1:1, C, 100°, 0.5, 28, -, Ph, m-C₆H₄Me, Et, Me, 1:1, C, 100°, 0.5, 77, 136°; Ph, m-C₆H₄Me, Et, Et, 1:2, A, -, 3, -, -, Ph, p-C₆H₄Me, Me, Me, 1:2, A, -, 3, 77, 146°; Ph, p-C₆H₄Me, Et, Et, 1:2, B, -, 3, 75, 152°; Ph, 2,4,1-Me₂C₆H₃, Me, Me, 2:1, A, -, 3, 83, 152°; Ph, 2,4,1-Me₂C₆H₃, Me, Et, 2:1, A, -, 3, -, -, Ph, 2,4,1-Me₂C₆H₃, Et, Et, 2:1, A, -, 3, 83, 146°; Ph, p-MeOC₆H₄, Et, Et, 1:2, B, -, 3, 81, 161°; Ph, p-MeOC₆H₄, Pr, Me, 1:2, C, 155°, 0.5, 55, 163°; Ph, m-O₂NC₆H₄, Me, Me, 1:2, C, 140°, 0.5, 62, 159°; Ph, m-O₂NC₆H₄, Me, Et, 1:2, C, 140°, 0.5, 34, -, Ph, m-O₂NC₆H₄, Et, Me, 1:2, C, 140°, 0.5, 24, 160°; Ph, m-O₂NC₆H₄, Et, Et, 1:2, C, 140°, 0.5, 38, -, Ph, 1-C₁₀H₇, Me, Et, 1:2, A, -, 3, 64, 174°; Ph, 2-C₁₀H₇, Me, Et, 1:2, A, -, 3, 50, 189°; Ph, 2-C₁₀H₇, Et, Et, 1:2, A, -, 3, 40, 184°; Ph, o-C₆H₄Cl, Me, Et, 2:1, A, -, 3, 13, 151°; Ph, o-C₆H₄Cl, Et, Et, 2:1, C, 170°, 0.5, 32, 192°; Ph, m-C₆H₄Cl, Me, Me, 1:1, C, 150°, 0.5, 35, 152°; Ph, p-

C6H4Cl, Et, Et, 1:2, C, 185°, 0.5, 59, 148°; Ph, p-C6H4Cl, Pr, Me, 1:2, C, 185°, 0.5, 37, 154°; Ph, Et, Et, 1:2, B, -, 3, 73, 82°; Ph, Et, Me, Et, 1:2, B, -, 3, 51, 118°; o-C6H4Me, Ph, Me, Me, 2:1, A, -, 3, 80, 112°; o-C6H4Me, Ph, Et, Et, 2:1, A, -, 3, 74, 137°; p-C6H4Cl, Ph, Et, Et, 1:2, C, 155°, 0.5, 67, 146°; p-C6H4Cl, Ph, Pr, Me, 1:2, C, 155°, 0.5, 21, 151°; 3,4,5-(MeO)3C6H2, Ph, Me, Me, 1:2, A, -, 3, 20, 181°; 3,4,5-(MeO)3C6H2, Ph, Et, Et, 1:2, A, -, 3, 37, 129°. The synthesis of I was modified by preparing II by rearrangement of ketoximes (IV) with PC15. The following procedures were used. A solution of IV (0.01 mole) in 50 cc. CHCl3 was treated at 0° with 0.01 mole PC15, the whole shaken 1-2 min., and the solution treated by one of the following procedures. The solution refluxed 15 min. to complete the rearrangement of IV, the III (0.02-0.03 mole) added in 10 cc. CHCl3, and reflux continued 2-3 hrs. (method D). Alternatively, the solution after remaining 2 hrs. at room temperature was cooled to 10°, the III (0.02-0.03 mole) in 10 cc. CHCl3 added, and the mixture left 1-2 days at room temperature (method E). The following method (F) gave good yields of I. The solution of rearranged IV, after 2 hrs. at room temperature was distilled at 40-5°/30 min., then stored 1-2 days with 0.02-0.03 mole III, and the products treated as previously described. I were crystallized as colorless needles from MeOH or alc. The following results were obtained (IV, R' in III, method, % yield, and m.p. of I given): PhMeC:NOH, Et, E, 65, 126°; (p-MeC6H4)MeC:NOH, Et, E, 65, 82°; (p-MeC6H4)MeC:NOH, Me, D, 65, 146°; 2-ClOH7CMe:NOH, Et, F, 65, 130°; PhPrC:NOH, Et, E, 72, 106°; PhPrC:NOH, Me, E, 35, 73°; (p-MeC6H4)2C:NOH, Me, F, 73, 128°; (p-MeC6H4)2C:NOH, Et, F, 60, 140°; Ph2C:NOH, Et, D, 55, 157°. Improved yields of I were obtained by using excess II or III.

RX(2) OF 2 D + E ==> F

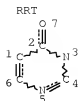


RX(2) RCT D 15999-95-8, E 42805-39-0
 PRO F 110244-33-2
 SOL 67-66-3 CHCl3
 NTE Classification: Heterocycle formation; Condensation;
 N-Acylation; # Conditions: CHCl3 20 deg 1-2days; # Comments:
 chloroimine reactant not isolated

FILE 'HOME' ENTERED AT 11:20:11 ON 13 DEC 2007

SEARCH HISTORY

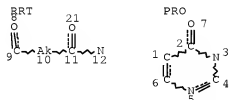
=> d stat que l35; d stat que l40;d his nofile
 L7 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
 L10 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

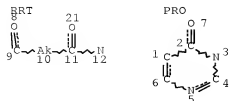
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 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

MAPPINGS

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|---------|-----|---------|-----|
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| 12 N | RRT | 3 N | PRO |

L11 STR



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

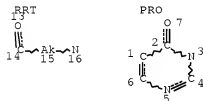
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 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
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| 12 | N | RRT | 5 | N | PRO |

L12 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

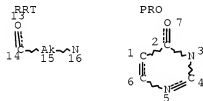
GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
| 3 | N | PRO | 16 | N | RRT |
| 16 | N | RRT | 3 | N | PRO |

L13 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 5 N | PRO | 16 N | RRT |
| 16 N | RRT | 5 N | PRO |

L14 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

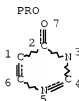
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 3 N | PRO | 19 N | RRT |
| 19 N | RRT | 3 N | PRO |

L15 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

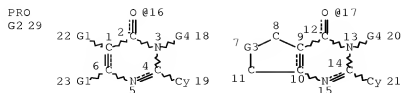
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 5 N | PRO | 19 N | RRT |
| 19 N | RRT | 5 N | PRO |

L18 1017 SEA FILE=CASREACT SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR
L15) NOT L7 (7766 REACTIONS)
L31 STR



Ak @24 Cy @28



```

VAR G1=H/X/CN/CF3/24/CB
VAR G2=16/17
REP G3=(1-3) C
VAR G4=H/24/25/28
REP G5=(0-1) CH2
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 24
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 19
GGCAT IS UNS AT 21
GGCAT IS LOC AT 24
GGCAT IS UNS AT 27
GGCAT IS UNS AT 28
DEFAULT ECLEVEL IS LIMITED

```

```

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

```

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STEREO ATTRIBUTES: NONE
L35 13 SEA FILE=CASREACT SUB=L18 SSS FUL L31 ( 67 REACTIONS)

```

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100.0% DONE 7766 VERIFIED 67 HIT RXNS 13 DOCS
SEARCH TIME: 00.00.01

```

L7 STR



```

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

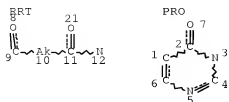
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

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STEREO ATTRIBUTES: NONE
L10 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

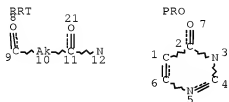
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

MAPPINGS

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|-----|-----|-----|-----|-----|-----|
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| 12 | N | RRT | 3 | N | PRO |

L11 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

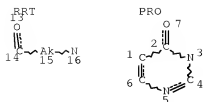
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
| 5 | N | PRO | 12 | N | RRT |
| 12 | N | RRT | 5 | N | PRO |

L12 STR



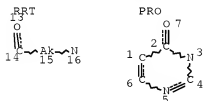
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 3 N | PRO | 16 N | RRT |
| 16 N | RRT | 3 N | PRO |
| L13 | STR | | |



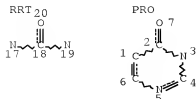
NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

****MAPPINGS****

| NOD SYM | ROL | NOD SYM | ROL |
|---------|-----|---------|-----|
| 5 N | PRO | 16 N | RRT |
| 16 N | RRT | 5 N | PRO |
| L14 | STR | | |



NODE ATTRIBUTES:
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 DEFAULT ECLEVEL IS LIMITED

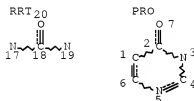
GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
| 3 | N | PRO | 19 | N | RRT |
| 19 | N | RRT | 3 | N | PRO |

L15 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

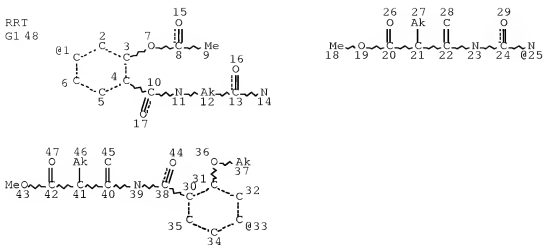
STEREO ATTRIBUTES: NONE

MAPPINGS

| NOD | SYM | ROL | NOD | SYM | ROL |
|-----|-----|-----|-----|-----|-----|
| 5 | N | PRO | 19 | N | RRT |
| 19 | N | RRT | 5 | N | PRO |

L18 1017 SEA FILE=CASREACT SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR L15) NOT L7 (7766 REACTIONS)

L37 STR



VAR G1=1/25/33

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 12

CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 37

CONNECT IS E1 RC AT 46

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 12

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L40 4 SEA FILE=CASREACT SUB=L18 SSS FUL L37 (13 REACTIONS)

100.0% DONE 87 VERIFIED

13 HIT RXNS

4 DOCS

SEARCH TIME: 00.00.01

(FILE 'HOME' ENTERED AT 10:13:21 ON 13 DEC 2007)

FILE 'CAPLUS' ENTERED AT 10:13:35 ON 13 DEC 2007

E US2005-551920/APPS

E US2006-551920/APPS

L1 1 SEA ABB=ON US2006-551920/AP

D SCAN

SEL RN

FILE 'REGISTRY' ENTERED AT 10:14:15 ON 13 DEC 2007

L2 39 SEA ABB=ON (116046-53-8/BI OR 128095-14-7/BI OR 1583-88-6/BI
OR 1655-07-8/BI OR 21615-34-9/BI OR 22396-14-1/BI OR 404-70-6/BI
OR 51756-10-6/BI OR 52721-69-4/BI OR 5538-51-2/BI OR
607-97-6/BI OR 609-14-3/BI OR 611-10-9/BI OR 64-04-0/BI OR
780771-35-9/BI OR 780771-36-0/BI OR 780771-37-1/BI OR 780771-38
-2/BI OR 780771-39-3/BI OR 780771-40-6/BI OR 780771-41-7/BI OR

780771-42-8/BI OR 780771-43-9/BI OR 780771-44-0/BI OR 780771-45-1/BI OR 780771-46-2/BI OR 780771-47-3/BI OR 780771-48-4/BI OR 780771-49-5/BI OR 780771-50-8/BI OR 780771-51-9/BI OR 780771-52-0/BI OR 780771-54-2/BI OR 780771-55-3/BI OR 780771-56-4/BI OR 780771-57-5/BI OR 780771-58-6/BI OR 85796-29-8/BI OR 916335-88-1/BI)
D SCAN

FILE 'STNGUIDE' ENTERED AT 10:19:14 ON 13 DEC 2007

FILE 'REGISTRY' ENTERED AT 10:34:32 ON 13 DEC 2007

L3 STR
L4 50 SEA SSS SAM L3

FILE 'CASREACT' ENTERED AT 10:35:14 ON 13 DEC 2007

L5 STR L3
L6 18 SEA SSS SAM L5 (274 REACTIONS)
L7 STR L3
L8 10 SEA SSS SAM L5 NOT L7 (161 REACTIONS)
D QUE
L9 STR L5
L10 STR L5
L11 STR L10
L12 STR L5
L13 STR L12
L14 STR L5
L15 STR L14
L16 5 SEA SSS SAM (L10 OR L11 OR L12 OR L13 OR L14 OR L15) NOT L7 (18 REACTIONS)
D QUE
L17 22744 SEA SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR L15) NOT L7 (419109 REACTIONS) EXTEND
L18 1017 SEA SSS FUL (L10 OR L11 OR L12 OR L13 OR L14 OR L15) NOT L7 (7766 REACTIONS)
SAVE TEMP JAI920CASRE/A L18
L19 957 SEA ABB=ON L18/COMPLETE
SAVE TEMP L19 JAI920CASRE2/A
L20 0 SEA ABB=ON US2006-551920/AP
L21 29 SEA ABB=ON SHCHERBAKOVA I?/AU
L22 0 SEA ABB=ON BALANDRIA M?/AU
L23 101 SEA ABB=ON HUANG G?/AU
L24 5 SEA ABB=ON GEOFFROY O?/AU
L25 116 SEA ABB=ON FOX J?/AU
L26 50 SEA ABB=ON NAIR S?/AU
L27 3 SEA ABB=ON (L21 OR L22 OR L23 OR L24 OR L25 OR L26) AND L19
D SCAN TI
L28 1 SEA ABB=ON TETRASUB?/TI AND L27
D BIBI
L29 7 SEA ABB=ON BALANDRIN M?/AU
L30 3 SEA ABB=ON (L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L29) AND L19
STR
L31 0 SEA SUB=L19 SSS SAM L31 (0 REACTIONS)
L32 0 SEA SUB=L18 SSS SAM L31 (0 REACTIONS)
L33 1017 SEA SUB=L18 SSS FUL L31 (7766 REACTIONS) EXTEND
L34 13 SEA SUB=L18 SSS FUL L31 (67 REACTIONS)
L35 SAVE TEMP L35 JAI920CASRE3/A
L36 3 SEA ABB=ON L35 AND L30

FILE 'STNGUIDE' ENTERED AT 10:56:32 ON 13 DEC 2007

FILE 'REGISTRY' ENTERED AT 11:05:59 ON 13 DEC 2007

FILE 'CASREACT' ENTERED AT 11:06:02 ON 13 DEC 2007

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L37      STR
L38      0 SEA SUB=L18 SSS SAM L37 (      0 REACTIONS)
L39      17 SEA SUB=L18 SSS FUL L37 (      87 REACTIONS) EXTEND
L40      4 SEA SUB=L18 SSS FUL L37 (      13 REACTIONS)
          SAVE TEMP L40 JAI920CASRE4/A
L41      13 SEA ABB=ON  (L35 OR L40)
L42      3 SEA ABB=ON  L30 AND L40
L43      720 SEA ABB=ON  L19 AND (PY<2003 OR AY<2003 OR PRY<2003)

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FILE 'STNGUIDE' ENTERED AT 11:15:58 ON 13 DEC 2007

FILE 'CASREACT' ENTERED AT 11:18:27 ON 13 DEC 2007

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L44      10 SEA ABB=ON  L41 NOT L30
L45      9 SEA ABB=ON  L44 AND L43

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FILE 'CASREACT' ENTERED AT 11:19:12 ON 13 DEC 2007

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D QUE NOS L30
D IBIB ABS FHIT L30 1-3

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FILE 'CASREACT' ENTERED AT 11:19:46 ON 13 DEC 2007

```

D STAT QUE L35
D STAT QUE L40
L46      10 SEA ABB=ON  (L35 OR L40) NOT L30
          D IBIB ABS FHIT L46 1-10

```

FILE 'HOME' ENTERED AT 11:20:11 ON 13 DEC 2007

```

D STAT QUE L35
D STAT QUE L40

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=>